This folder contains files that will come in hand for running multiple runs of HOLE on a ion channel protein. The steps to be followed are as follows:

Step 1: Open *hole.inp* and replace *pdbfilename.pdb* with the name of your pdb file.

```
! note that HOLE input
coord pdbfilename.pdb
radius ~/hole2/rad/simp
        ! n.b. can use
```

Step 2 (optional): You can modify the radius values the program uses to run the calculations by modifying the selection called *simple.rad*.

```
coord pdbfilename.pdb           ! Co-ordinates in pdb format
radius ~/hole2/rad/simple.rad ! Use simple AMBER vdw radii
        ! n.b. can use ~ in hole
```

Step 3: Save the file *hole.inp.* Open terminal and run the command:

```
pgupta@mems13:.../AutomationScripts/HoleAutomation$
expect script_100ROUNDS.exp
```

Step 4: The terminal will start running the HOLE calculations. Leave it undisturbed for ~10mins.

Step5: Once the calculations have completed, open the file holeshow2.tcl.

Step 6: Replace the prot.pdb name with your pdb file's name. Save the file and close it.

```
proc loadh {j} {
set k [expr $j+100]
for {set i $j} {$i<$k} {incr i} {
mol new prot.pdb
mol delrep 0 top
```

Step 7: Open terminal and launch VMD. Once vmd has loaded, enter "source holeshow2.tcl" in the terminal window and press enter.

Step 8: Next, type "loadh 1" to load 10 runs of the HOLE calculations starting from Run 1. Replace the number 1 with a number X to load runs X to X+9.

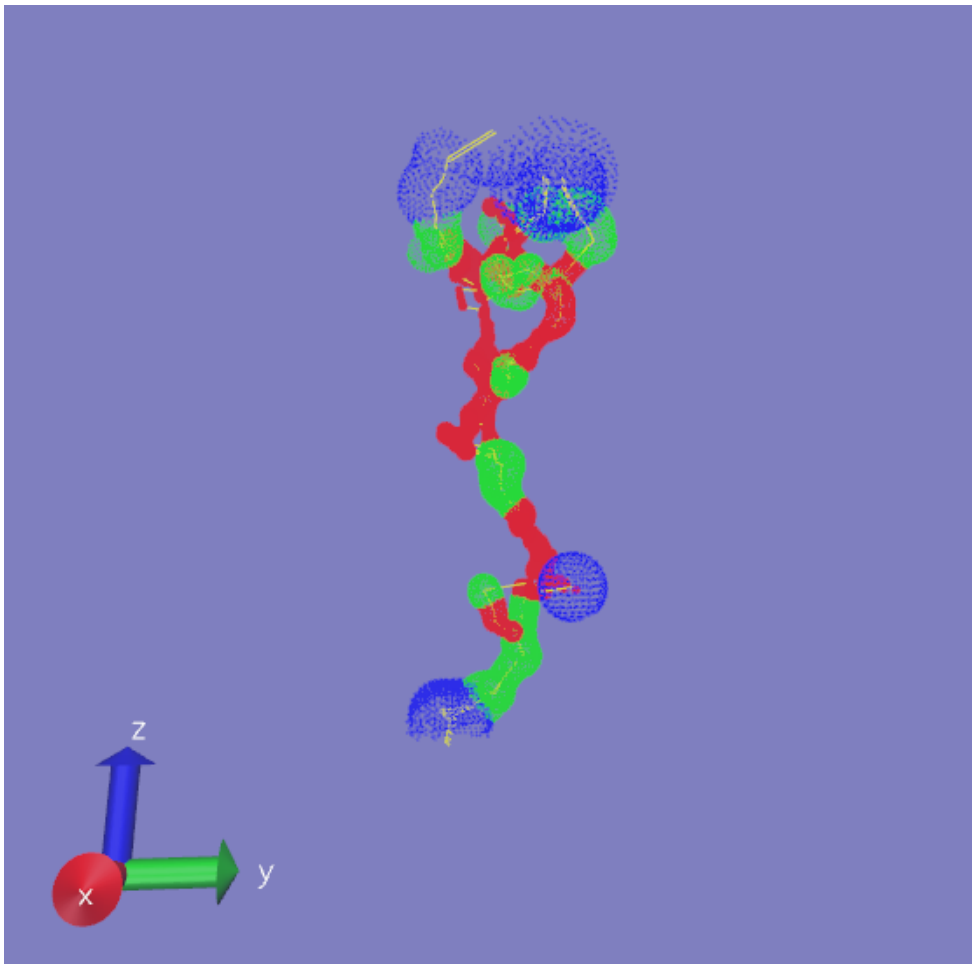

Fig. *(right)*
A view of the output of 10 runs displayed simultaneously using the *loadh* command supplied to VMD via holeshow2.tcl.